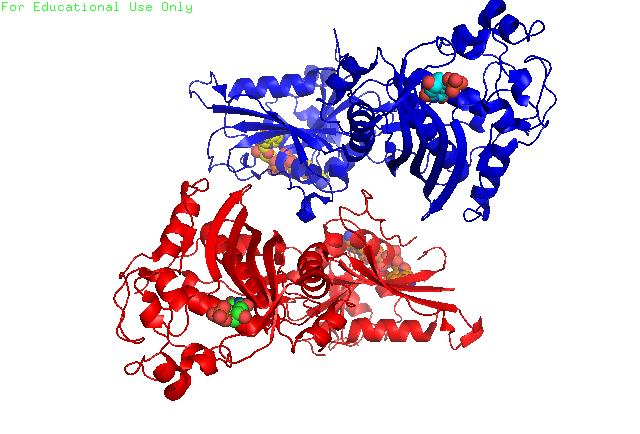
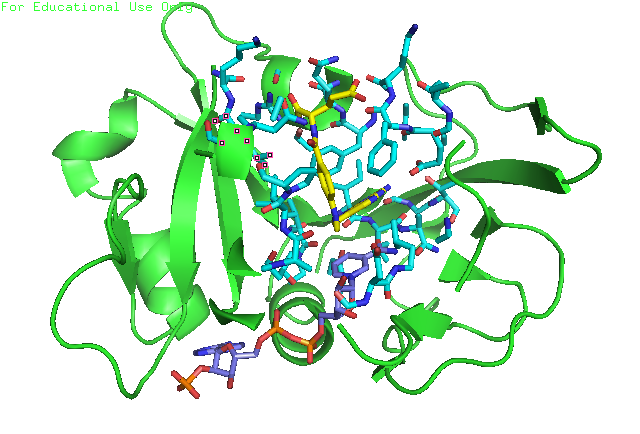
Pymol Refresher



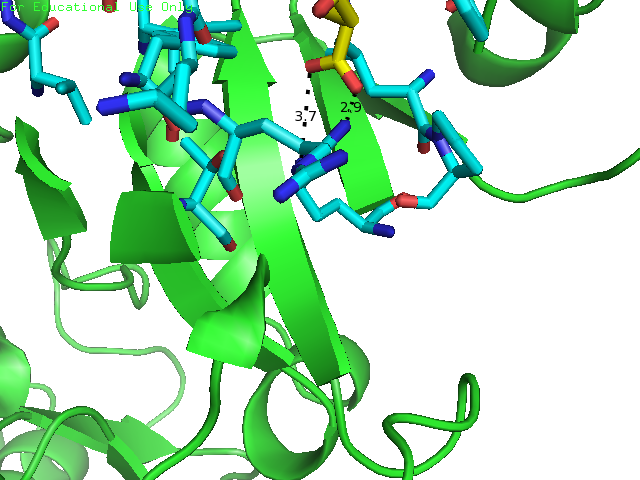
The protein 2H2Q is shown to the left with hydrophobic residues in pink, hydrophilic residues in yellow, and ionic residues in red.



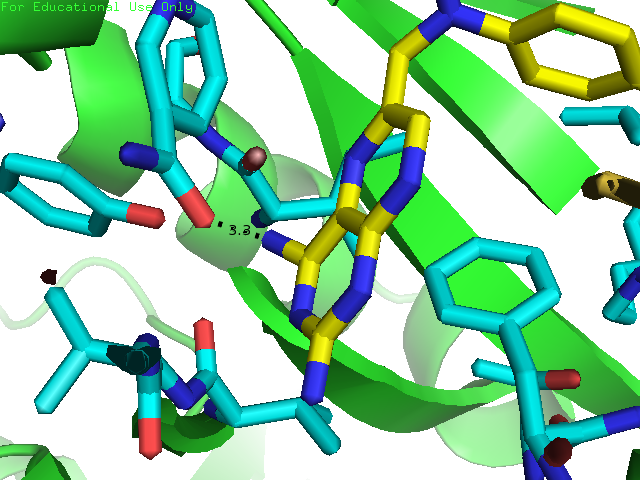
The protein 2H2Q is shown to the left with subunit 1 is shown as a cartoon in blue, with NAD in yellow carbons as spheres and DP in light blue carbons. The subunit 2 is shown in red as a cartoon with orange NAD and green DP shown as spheres.



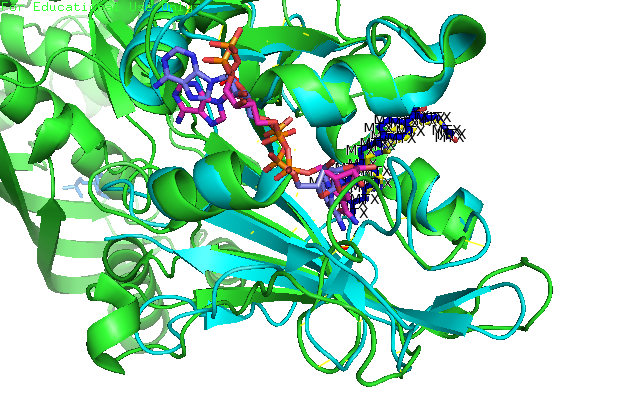
The enzyme 3CL9 is shown to the left with the active site in light blue carbons as sticks. MTX is shown with yellow carbons as sticks, and NAD is shown in dark blue carbons as sticks.



The protein 3CL9 is shown to the left with hydrogen bonds between MTX (yellow carbons) and the active site of the protein (light blue carbons)

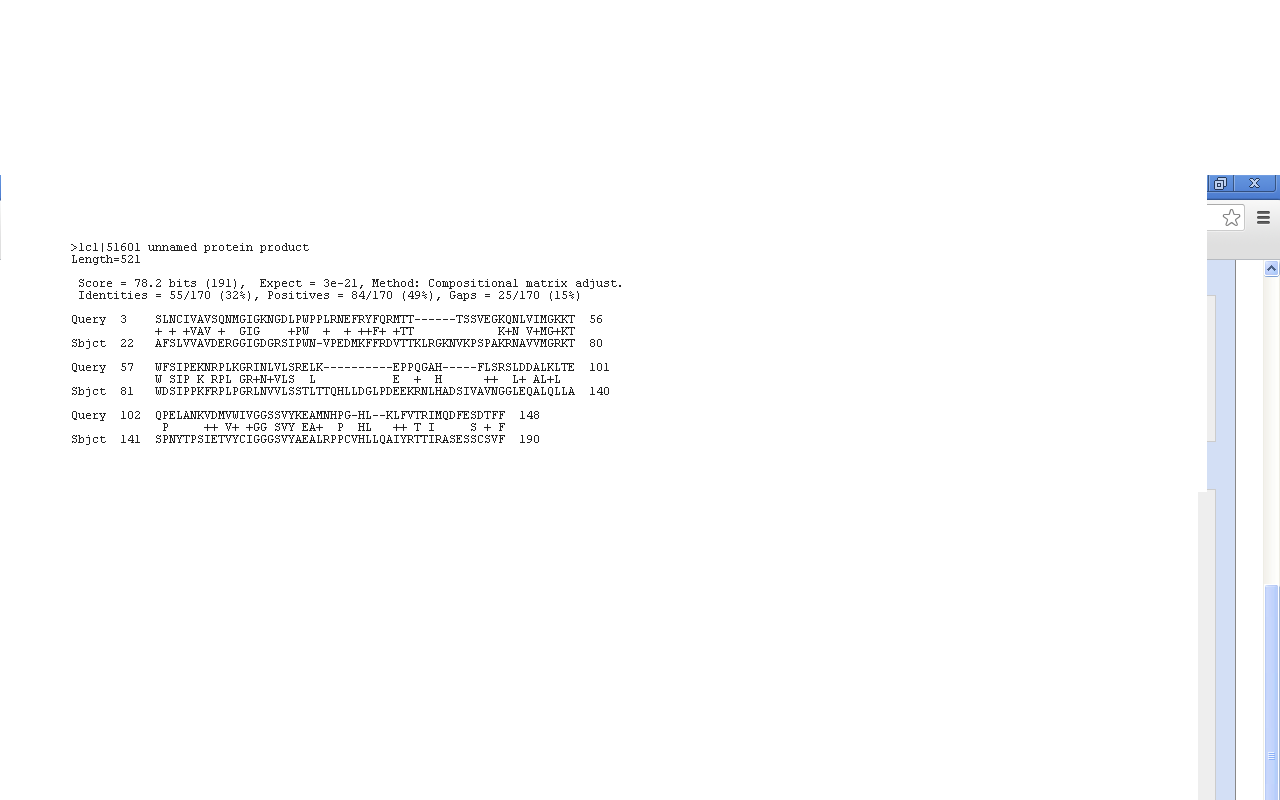


The protein 3CL9 is shown to the left with hydrogen bonds between MTX (yellow carbons) and the active site of the protein (light blue carbons)

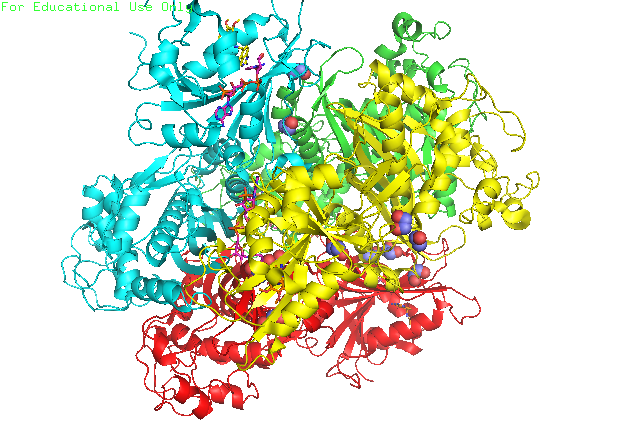


The protein 3CL9 (green) is aligned 1U72 (light blue), the substrates are shown as sticks. 3CL9 MTX is dark blue, and NAD is in purple. 1U72 MTX is yellow and NAD is pink.

The RMS value is 1.126 111-111 atoms. The 2 molecules are 78% similar.



The pair wise comparison of the proteins is shown above. Human DHFR is much smaller than the T. cruzi.



The protein 3HBB with A (blue), B(green), C (yellow), and D (red) subunits are displayed. MTX is in orange sticks and NAD is in pink sticks. EDO is shown in blue spheres.

Valine, alanine, and isoleucine are common to the active sites.